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SWAT—A Semi-empirical Model to Predict Concentrations of Pesticides Entering Surface Waters from Agricultural Land

Colin D. Brown* & John M. Hollis

Soil Survey and Land Research Centre, Cranfield University, Silsoe, Beds, MK45 4DT, UK

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Abstract: A semi-empirical model called SWAT has been developed to predict concentrations of agriculturally applied pesticides moving to surface waters, an aspect which is not well described by current models for pesticide fate. The model is based upon a direct hydrological link established between soil type and the amount of water moving rapidly to streams in response to rainfall. Attenuation factors describe the decrease in concentrations of pesticide between field application and loss in water moving from the site into surface waters. Evaluation of model predictions against available field data from three sites and four soil types in England shows that SWAT is capable of predicting the transient peak concentrations of a wide range of pesticides during rapid water movement to streams in response to rainfall. Predicted concentrations were too great when rainfall initiated water movement to streams very soon after pesticide application, particularly for the more mobile pesticides, and some predictions for pesticides sorbed very strongly to soil were relatively poor. Almost all of the predicted concentrations were within one order of magnitude of measured values.

Key words: mathematical model, pesticide, surface waters, contamination, evaluation.

1 INTRODUCTION

Mechanistic models of pesticide leaching use the Richards' and convection-dispersion equations to describe movement through the soil profile, whilst simpler, management models often treat water flow *via* a 'tipping-bucket' mechanism. Losses of pesticide in surface run-off have been modelled in the USA using the SCS curve number approach combined with the Universal Soil Loss Equation.[1,2] A number of soil processes can, under certain circumstances, result in the failure of these models adequately to simulate observed behaviour, including bypass flow,[3] movement to surface waters *via* drainage systems[4] and lateral flow through rather than across the soil.[5] One or more of these processes often makes a significant contribution to pesticide transport to surface waters in the UK and there is a need for a more generally applicable model which is robust enough to cope with a variety of combinations of soil, climate, pesticide and management practices. Two approaches to the description of complex phenomena observed in the field are possible. First, modellers can draw upon knowledge for all of the processes to be described and incorporate this into a model which adopts a rigorous approach to describe real life as fully as possible. A drawback of such models can be the inclusion of a large number of parameters, some of which may not be directly measurable or may not be available for a given situation. The alternative approach, and that taken by the model presented in this paper, is to use a number of simplifying assumptions to allow a generalised description of a range of processes.

* To whom correspondence should be addressed.

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The paper will describe the concepts of SWAT, an attenuation model describing the movement of pesticides to surface waters which was previously outlined by Hollis,[6] and then evaluate the performance of the model against field data collected in the UK.

2 MODEL CONCEPTS

The hydrological component of the SWAT model is based upon a direct, empirically derived link between soil type and stream response to rainfall which has been reported as the Hydrology Of Soil Types (HOST) system.[7] This system groups all soil series recognised in the UK into one of 29 classes based upon the hydrological characteristics of the soil and underlying substrate layer. The 29 classes have been calibrated against measured stream flow characteristics for 800 catchments across the UK.[8] Each soil hydrological class is related to a stream-flow coefficient using multiple regression based on the proportion of HOST classes in each catchment and the measured coefficient for that catchment. The two principal stream-flow coefficients used are termed standard percentage run-off (SPR) and base flow index (BFI). SPR is defined as that proportion of rainfall which causes a short-term increase in stream-flow over the first 24-h period after a storm event and the measured values for this parameter range from 3·8 to 77·5% for 200 catchments in the UK. BFI is that fraction of the long-term total stream volume which is represented by base flow and has measured values of approximately 0·15 to 0·95 for 575 catchments in the UK, although predicted values have a maximum of 1·0. Using the HOST system, soils in England and Wales have been grouped into five hydrologically distinct classes for soil run-off potential, S1 to S5, based on their predicted SPR and BFI coefficients (Table 1). S1 soils show the largest stream responses to rainfall (largest standard percentage run-off and smallest base flow index) and S5 soils show the smallest response. Those soils with the largest predicted response coefficients are the most sensitive to rainfall and require only small amounts before stream response is initiated. Conversely, soils with the smallest predicted response coefficients require large amounts of rain to induce response. The five classes for soil run-off potential form the basis for SWAT predictions of the movement of water and associated pesticide to streams in response to rainfall events.

A 'minimum standard rainfall volume', R, has been defined as that required to induce stream response for each of the classes for soil run-off potential (Table 1). No water from a soil is predicted to contribute to stream response unless this amount of rainfall or more is received during a single event defined on a daily time-step. Calculation of the concentration of pesticide in soil water reaching surface water courses is then based upon the time, t, between application of the pesticide and the first rainfall event that equals or exceeds the minimum standard rainfall volume required to produce stream response.

Upon application, pesticide is assumed to penetrate to a depth of 2 mm. Subsequently, the pesticide will move down the soil profile such that in time, t, the depth penetrated, d (mm), can be defined by:

$$d = 2 + \{(t * K_{0\cdot05})/\mathrm{RF}\}, \quad (1)$$

where $K_{0\cdot05}$ is the hydraulic conductivity of the soil (mm day^{-1}) at a tension of 5 kPa and RF is a retardation factor which is dependent upon pesticide sorption and volatilisation. Calculation of the depth penetrated relies upon the assumption that the soil is at field capacity with a mean vertical recharge equal to the hydraulic conductivity at this water content. The retardation factor is defined by:

$$\mathrm{RF} = 1 + \{(K_d * \rho_b)/W_i\} + \{(C_a * K_H)/W_i\}, \quad (2)$$

where K_d is the partition coefficient of the pesticide between soil and water (ml g^{-1}), ρ_b is the bulk density of the topsoil (g cm^{-3}), C_a is the air capacity fraction of the topsoil,[9] K_H is Henry's constant for the pesticide, and W_i is the 'interactive' soil water fraction which is

TABLE 1
Stream-Flow Coefficients and Minimum Standard Rainfall Volumes Required to Induce Stream Response for Each Class for Soil Run-Off Potential in England and Wales

Run-off potential class	*Standard percentage run-off*	*Base flow index*	*Minimum standard rainfall volume (mm)*
S1	50–60	≦0·25	5
S2	40–60	0·26–0·40	7
S3	25–50	0·40–0·75	10
S4	2–30	0·76–0·95	18
S5	2	0·95–1·00	20

defined as the difference between the water content of the soil at 5 kPa tension and 50% of the water content at 1500 kPa tension. The interactive soil water fraction is hypothesised to be that fraction of the total soil water with which pesticide comes into contact and it excludes some strongly held water on the basis that diffusion in it would be very slow.[10]

At the time, t, of the event producing stream response, pesticide is assumed to be evenly spread throughout the top d mm of soil, with a concentration in soil water, C, which is given by:

$$C = (M_i/W_t) * \mathrm{PF}_t * \mathrm{AF}, \tag{3}$$

where M_i is the corrected rate of application of pesticide (g ha^{-1}), calculated as applied pesticide minus that proportion intercepted and retained by the crop, and W_t is the total volume of interactive water in the top d mm of soil (litre ha^{-1}). PF_t and AF are partition and attenuation factors to account for pesticide sorption and degradation, respectively, during time t. They can be defined by the equations:

$$\mathrm{PF}_t = 1/\{1 + (K_{dt} * \rho_b) + (C_a * K_H)\} \tag{4}$$

and,

$$\mathrm{AF} = e^{-kt}, \tag{5}$$

where K_{dt} is a time-dependent partition constant between soil water for the pesticide (ml g^{-1}) and k is the first-order degradation coefficient (day^{-1}).

K_{dt} is included to take account of observations that the proportion of pesticide in the sorbed phase often increases with time. In the absence of experimental data, K_{dt} is defined (after Walker[11]) as:

$$K_{dt} = K_d\{1 + (0{\cdot}1 * t^{0{\cdot}5})\} \tag{6}$$

At time t, rainfall infiltrates the soil and a proportion of the rainfall, equal to the 'minimum standard rainfall volume', R (see Table 1) is hypothesised to displace and mix with the mobile soil water fraction in the top 1 mm of soil. This effectively dilutes the concentration of pesticide in the displaced mobile water fraction by a dilution factor, DF:

$$\mathrm{DF} = W_m/R \tag{7}$$

where W_m is the mobile soil water fraction in the top 1 mm of soil which is assumed to move during leaching and is defined as the difference between the water content of the soil at 5 and 200 kPa tension.[10]

The displaced mobile soil water fraction, now mixed with the minimum standard rainfall volume, is then assumed to move to surface waters, either *via* 'bypass' flow through the soil to drains, topsoil lateral throughflow, or overland flow. Finally, pesticide in water moving to surface waters will be subject to some sorption to soil as it moves. This is accounted for empirically by reducing concentrations of pesticide in the soil mobile water/rainfall mixture by applying a partition factor, PF, which is independent of time and can be obtained by replacing K_{dt} by K_d in eqn (4) above.

Thus the concentration of pesticide impacting at the nearest surface water, DC, is defined by:

$$\mathrm{DC} = C * \mathrm{DF} * \mathrm{PF}. \tag{8}$$

Using eqns (1) to (8), the SWAT model can be run to predict the maximum concentration of pesticide in waters impacting on surface water courses during peak stream-flow in response to rainfall in one of two ways:

(a) at the local catchment or sub-catchment scale, using measured rainfall data to simulate peak concentrations reaching surface waters in response to individual rainfall events; and
(b) at the regional or national scale, using climatic data to estimate the likelihood of a 'minimum standard rainfall volume' occurring within a specific period after pesticide application; a methodology incorporating such broad extrapolation has previously been described.[6]

3 MODEL EVALUATION WITH FIELD DATA

The hydrological component of SWAT is based upon work to develop the hydrological classification, HOST, for soils in the UK.[7] This involved the analysis of flow data from approximately 800 catchments around the UK to examine the relationship between hydrological variables and soil hydrological class. For the two hydrological variables used to derive classes for soil run-off potential, the predicted stream-flow coefficients explained 80 and 60% of the measured variation in BFI and SPR, respectively.[8] No further validation of the classes for soil run-off potential used in SWAT is considered necessary unless, for example, they are to be extrapolated to other countries. This section will thus only consider the ability of SWAT to predict concentrations of a range of pesticides moving to surface waters in the UK.

The most appropriate data for evaluating a semi-empirical model such as SWAT are for movement of pesticides to surface waters at the field scale. Over the past few years, a number of field experiments in the UK have monitored such movement and data collected at Rosemaund, Herefordshire, Temple Balsall, Warwickshire and Cockle Park, Northumberland have been

TABLE 2
Soils Parameters Used to Model the Movement of Pesticides to Surface Waters at Rosemaund and Temple Balsall (Water Contents are Volumetric)

		Temple Balsall		
Parameter	*Rosemaund*	*Sandy loam*	*Clay loam*	*Cockle Park*
Soil series	Bromyard	Hall	Brockhurst	Dunkeswick
Topsoil organic carbon (%)	1·66	3·20	2·30	3·27
Topsoil bulk density (g cm^{-3})	1·21	1·45	1·37	1·12
Topsoil total porosity fraction	0·531	0·463	0·480	0·540
Topsoil water fraction: 5 kPa	0·396	0·263	0·354	0·403
Topsoil water fraction: 200 kPa	0·239	0·163	0·299	0·280
Topsoil water fraction: 1500 kPa	0·175	0·105	0·176	0·192
Topsoil hydraulic conductivity at 5 kPa (mm day^{-1})	13·4	4·5	8·9	8·9

used to evaluate critically the performance and broader applicability of SWAT at the local sub-catchment scale. The data selected cover 15 individual pesticides, four different soil series, and three of the five classes for soil run-off potential. Literature values for the mean half-lives of the pesticides in soil range from 10 to 400 days and representative values for K_{oc} range from 10 to 8000 ml g^{-1}.[12,13] The soils are a silty clay loam at Rosemaund, a clay loam and a sandy loam at Temple Balsall, and a clay loam at Cockle Park.

3.1 Field experimental datasets

Rosemaund is an ADAS Research Centre in Herefordshire which encompasses an entire small water catchment that ultimately drains into the River Lugg. A collaborative programme to measure the dispersion of pesticides from the catchment into the stream ran from Autumn 1987 to Spring 1994.[14,15] A total of 11 different pesticides were applied over a period of five years to two fields at Rosemaund known as Foxbridge & Longlands and Stoney & Brushes. Soils are largely silty clay loams, with the Bromyard, Bromyard shallow phase, Middleton and Compton series all represented. Of these, the Bromyard series predominates, and this series was used as the basis for modelling the site. Pesticide concentrations were monitored in drainage ditches and in the stream for which Rosemaund makes up almost 100% of the catchment. Monitoring was event-based, so that relatively large numbers of samples were collected over short periods at irregular intervals. From each batch of samples, the maximum concentration observed was selected for comparison with predictions from the model, as it is this concentration which SWAT should best simulate. In addition, the median concentration of samples taken over an event was calculated to compare model results with concentrations impacting upon surface waters over a broader time-scale. The median was preferred over the mean to take account of results quoted as being below the limit of detection for the analytical method.

At Temple Balsall, Warwickshire, data on the mobility of three pesticides were collected in a series of studies for Monsanto Agricultural Company.[16,17] In the last of these studies, the environmental fates of alachlor, atrazine and pendimethalin were compared following application in spring to a fodder maize crop. Pesticide movement was monitored for two contrasting soil types at a single site with a sandy loam soil of the Hall series and a clay loam soil of the Brockhurst series present within the same field. Samples of overland flow were collected using 1-m^2 traps and movement to depth was evaluated by collecting samples of soil water after major rainfall events using suction samplers. Water samples were stored refrigerated (4–6°C) in amber glass bottles until analysis for pesticide content by Corning Hazleton, Harrogate, UK. Samples (250 ml) were concentrated and cleaned up by passing through a C18 Polar plus Bakerbond SPE cartridge which was subsequently eluted with iso-octane + ethyl acetate (4 + 1 by volume; 5 ml). The eluant was evaporated to dryness under nitrogen, resuspended in iso-octane + ethyl acetate (1 ml), and the three compounds were analysed by GCMS. The limit of determination for all three pesticides was 0·05 μg $litre^{-1}$ and mean recoveries from three samples spiked to 1·0 μg $litre^{-1}$ were 62, 87 and 76% for alachlor, atrazine and pendimethalin, respectively.

Water and associated solutes moving to depth from the sandy loam soil would generally be expected to reach groundwater rather than surface waters, so that only data collected for overland flow were compared with model predictions. By contrast, overland flow from the Brockhurst soil combines with flow from drains (where installed) to give the total impact upon surface waters which is simulated by SWAT. In order to take account of this, data for concentrations of pesticide in overland flow and soil water at drain depth (80 cm) were combined for any given sampling date. A ratio of

TABLE 3
Pesticide Parameters Used to Predict Movement to Surface Waters from the Rosemaund and Temple Balsall Sites (* indicates Measured, Site-Specific Value)

Pesticide	K_{oc} (*ml* g^{-1})	*Field half-life* (*day*)	*Henry's constant* (*atm-m*^{3} *mole*$^{-1}$)
Rosemaund			
2,4-D	20	10	$1{\cdot}1 \times 10^{-7}$
Dicamba	2	14	$6{\cdot}3 \times 10^{-8}$
Dichlorprop	1000	10	0
Dimethoate	20	7	$1{\cdot}1 \times 10^{-9}$
Isoproturon	120	30	$5{\cdot}1 \times 10^{-9}$
Lindane	1100	400	$3{\cdot}2 \times 10^{-4}$
MCPA	20	25	$2{\cdot}0 \times 10^{-8}$
Mecoprop	20	10	$4{\cdot}4 \times 10^{-8}$
Oxydemeton-methyl	10	10	0
Simazine	130	60	$1{\cdot}3 \times 10^{-8}$
Triclopyr	780	46	$4{\cdot}0 \times 10^{-8}$
Temple Balsall: Hall soil/Brockhurst soil			
Alachlor	170/113*	23*/21*	$1{\cdot}3 \times 10^{-6}$
Atrazine	100/100	72*/86*	$1{\cdot}2 \times 10^{-7}$
Pendimethalin	5000/5000	107*/96*	$1{\cdot}5 \times 10^{-3}$
Cockle Park			
Isoproturon	120	30	$5{\cdot}1 \times 10^{-9}$
Trifluralin	8000	60	$3{\cdot}8 \times 10^{-3}$

7 : 1 drainflow to overland flow was estimated for the HOST class within which the Brockhurst series is grouped and this ratio was then used to produce a time series of weighted average concentrations from the two datasets.

Data from Cockle Park, Northumberland are from a collaborative project between the University of Newcastle upon Tyne and ADAS.[18,19] A pesticide experiment was established on an existing drainage trial on a clay loam soil of the Dunkeswick series and pesticides including isoproturon and trifluralin were applied to winter wheat in two successive seasons, of which 1990/91 was selected as the most comprehensively monitored. Losses of water and pesticides from a mole-drained plot in surface-layer flow through the top 30 cm of the soil profile and mole drainflow were monitored between November 1990 and March 1991. These two flow processes are described as a single loss mechanism by SWAT, so daily flow totals were combined and pesticide concentrations were adjusted according to rate of surface-layer flow and drainflow to give a single daily concentration representative of the total impact on adjacent surface waters.

3.2 Modelling parameters

Input parameters required by SWAT are fairly limited. Parameters for the four soil types modelled are given in Table 2. All are readily measured using standard techniques, apart from the hydraulic conductivity of soil at field capacity (taken as 5 kPa tension). This was predicted from the relationship between saturated hydraulic conductivity, estimated from its curvilinear relationship with air capacity,[20] unsaturated conductivity and water content, using pedotransfer functions based on the closed-form equation of Van Genuchten.[21] Van Genuchten's β and n parameters were estimated from non-linear regression equations incorporating bulk density and sand, silt, clay and organic carbon contents for a UK soil dataset.[22] An analysis of the sensitivity of model output to changes in the value selected for topsoil hydraulic conductivity at field capacity shows that predicted concentration of a given pesticide is approximately inversely, linearly related to hydraulic conductivity at field capacity within the expected range for this parameter in UK soils. Attention should be paid to the method of estimating or measuring this parameter.

The only climatological data required by the model are the minimum standard rainfall volumes required before movement to surface waters is initiated on the four soil types. Values for this parameter were selected according to the classification of the soil series into Runoff Potential classes as discussed in Section 2. The Bromyard, Hall, Brockhurst and Dunkeswick series belong to classes S3, S5, S2 and S2, respectively, resulting in defined minimum standard rainfall events of 10, 20, 7 and 7 mm, respectively. Measured rainfall for

each site was used to trigger run-off to surface waters on each day for which total rainfall exceeded the defined rainfall events above, with the total movement to surface waters calculated as the product of daily rainfall and standard percentage run-off value.

The predictive ability of the model was evaluated for circumstances in which little or no site-specific data on pesticide properties are available. Thus, measured values for compound input parameters were only available for some of the pesticides monitored at Temple Balsall. Literature databases[12,13,23] were used to select representative values for K_{oc}, half-life in soil and Henry's constant for the pesticides monitored at Rosemaund and Cockle Park (Table 3).

3.3 Comparison between model predictions and field data obtained at Rosemaund

Model results and field data are compared in Table 4 for 11 different pesticides monitored at Rosemaund between autumn 1987 and spring 1991. Where two times are given for a single event, concentrations of pesticide detected are attributable to two different applications of the same pesticide to different fields. Similarly, where two concentrations are given for a single events, the first value is for a field drain and the second value is for stream water.

Generally, the comparison between model results and field data was good, particularly given the absence of site-specific data for pesticide properties which are often the overriding factor in determining pesticide fate. There were three events monitored at Rosemaund where significant rain fell within five days of application of a pesticide and, for each of these events, the maximum concentration observed was over-predicted by the model. The three pesticides, MCPA, mecoprop and oxydemeton-methyl, are all relatively mobile and observed concentrations were over-predicted by factors of between 3 and 8. Thus predicted concentrations from SWAT were within an order of magnitude even for poorly simulated events, comparing favourably with the performance of other, more complex surface water models.[24] For all events occurring more than five days after compound application, the model underestimated the transient peak in pesticide concentrations observed

TABLE 4
Comparison between Observed and Predicted Concentrations of a Range of Pesticides in Drainflow and Stream Water at Rosemaund

Pesticide	*Application date*	*Application rate (g ha⁻¹)*	*Time from application to storm event (day)*	*Observed maximum concentration (μg litre⁻¹)*	*Observed median concentration (μg litre⁻¹)*	*Predicted concentration (μg litre⁻¹)*
2,4-D	20/11/87	1000	30	1·0	0·8	0·5
	08/12/88	600	79	<0·01	—	0
Dicamba	20/11/87	425	30	0·7	0·5	0·4
	08/12/88	255	79	<0·01	—	0
Dichlorprop	20/03/90	2600	58	1·0	0·5	0
Dimethoate	28/11/90	340	27	3·1	0·5	0·3
			41	0·58/0·22	0·15/0·02	0
Isoproturon	01/11/89	1000	8	8·4	1·8	6·8
			10	13·7	2·3	5·4
	17/11/89	375	27/43	8·8/5·4	4·0/5·0	1·7
			28/44	5·2/3·2	2·1/3·2	1·6
	11/10/90/	1000/	32/44	17·2	5·9	3·5
	23/11/90	2130	46/58	12·1/2·6	2·5/0·6	1·8
			90/102	2·1	0·7	0·4
Lindane	01/11/89	560	43	0·27	0·24	0·10
			44	0·29	0·09	0·10
			139	0·03	0·01	0·02
MCPA	28/02/91	1680	5	18·8/12·4	2·7/1·2	48·7
			16	12·7	0·5	10·4
Mecoprop	17/11/87	2000	2	11·7	1·5	89·6
			30	<0·1	—	0·4
	22/03/90	650	56	1·4	0·4	0
Oxydemeton-methyl	01/03/91	114	4	0·8	<0·15	5·4
			15	<0·15	—	0·7
Simazine	08/12/88	1150	79	1·8	0·4	0·3
Triclopyr	08/12/88	195	79	<0·01	—	0·01

in drain and stream waters at Rosemaund. However, all predicted concentrations were within an order of magnitude of observed maxima. For events occurring more than five days after application of a pesticide, model results were either very close to or over-predicted the median of observed data.

3.4 Comparison between model predictions and field data obtained at Temple Balsall

Figures 1 and 2 compare observed concentrations of alachlor, atrazine and pendimethalin with model predictions for the sandy loam (Hall) and clay loam (Brockhurst) soils, respectively. 'Observed' data for the Brockhurst soil are concentrations impacting upon

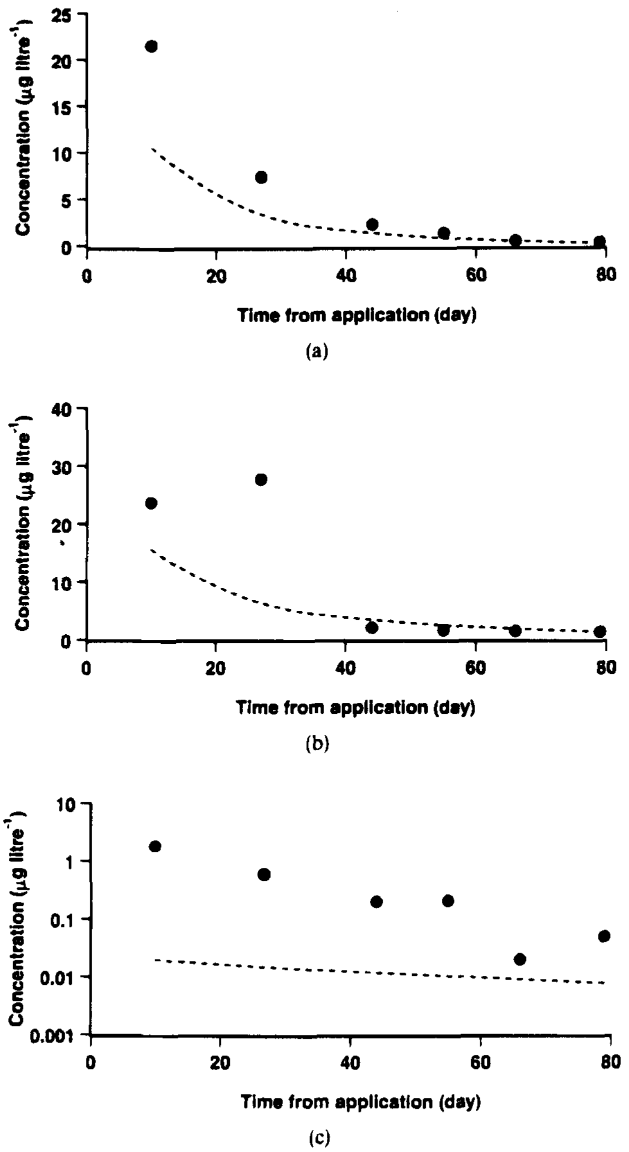

Fig. 1. Comparison between (●) observed concentrations entering surface waters from the sandy loam site at Temple Balsall and (---) those predicted by SWAT: (a) alachlor; (b) atrazine; and (c) pendimethalin.

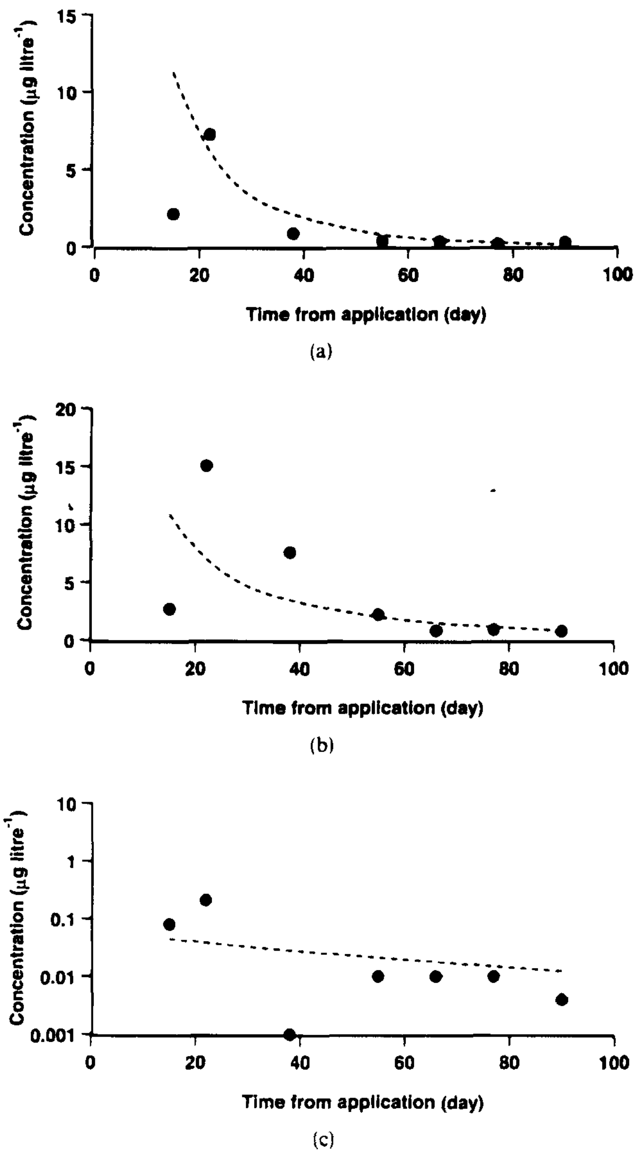

Fig. 2. Comparison between (●) observed concentrations entering surface waters from the clay loam site at Temple Balsall and (----) those predicted by SWAT: (a) alachlor; (b) atrazine; and (c) pendimethalin.

surface waters calculated from data for overland flow and soil water as described in Section 3·2. It should be noted that the y-axis for data on pendimethalin is logarithmic because of the small value of predicted and observed concentrations.

Overall, simulation of the movement of alachlor and atrazine to surface waters from both Hall and Brockhurst soils is good. Most data points fall within the range predicted by SWAT and the fairly rapid decrease in observed concentrations with time is well reproduced by the model. The main exception to this good fit is the first event after applications in the Brockhurst soil, where observed concentrations were up to five times smaller than predicted and factors other than those considered implicitly by the model would appear to be influencing the movement of pesticides.

Pendimethalin is very strongly sorbed to the soil (K_{oc} = 4000 ml g^{-1}) and concentrations predicted by SWAT did not closely match observed data. This was particularly true for the Hall soil where observed concentrations were generally at least an order of magnitude larger than the range of concentrations predicted by the model. Concentrations of pendimethalin measured in flow from the Brockhurst soil varied considerably and were under-predicted by the model in events soon after application and over-predicted in events later in the season. Movement of pesticide as the sediment-sorbed species would be expected to be a significant component of the total transport of pendimethalin to surface waters, although this total transport is small. Movement sorbed to sediment is not dealt with by SWAT and this may partially explain the lack of fit between observed and predicted data.

3.5 Comparison between model predictions and field data obtained at Cockle Park

Data on rates of surface-layer flow and drainflow at Cockle Park were available to complement pesticide data and this meant that the effects upon predictions for pesticide movement of the simplifying assumptions about soil hydrology in SWAT could be evaluated for the two contrasting pesticides, isoproturon and trifluralin. As described above, SWAT works by estimating the proportion of any given rainfall event which moves rapidly to adjacent surface waters within 24 h. The minimum standard rainfall event required to generate run-off from the Dunkeswick clay loam soil at Cockle Park is 7 mm. Thus, no loss of either water or pesticide will be predicted for any day where total rainfall is less than 7 mm. If rainfall of 7 mm or greater is received in a day, then the standard percentage run-off figure (45% for Dunkeswick) is used to calculate the amount of that rainfall moving to surface waters. The predictions of SWAT for peak flow in response to rainfall are compared with the combined daily totals of surface-layer and drainflow observed at Cockle Park in Fig. 3. Generally, timing of peaks in observed flow is well predicted by SWAT, although the actual magnitude of the peaks is underestimated. Several events are predicted in early February, but were not actually observed because the ground was frozen during this period. Similarly, a number of events were observed as snow thawed and the ground defrosted in mid-February and these are not predicted by SWAT because there was little incident rainfall.

Total flow over the winter of 1990/91 was 285·0 mm, whereas SWAT predicted that there would be 83·1 mm of rapid throughflow (29% of the total). The remainder of the observed flow is postulated by SWAT to be slower seepage water and the model assumes that this water will be relatively ineffective in transporting pesticide from the soil. The accuracy of this assumption is tested by comparing observed concentrations of isoproturon and trifluralin adjusted to reflect the total loss to surface waters with the concentrations predicted by SWAT (Figs 4 and 5). For trifluralin, which is strongly sorbed to soil (K_{oc} = 8000 ml g^{-1}), predictions from SWAT were reasonably accurate. With the exception of a single event in mid-January, concentrations of trifluralin in flow were only observed during periods when SWAT predicted that rapid through flow would be occurring. This reflects the fact that bypass flow is the only important pathway for such a strongly sorbed pesticide to be transported through soil to surface waters over its residence period in soil. The maximum observed concentrations were relatively well predicted by SWAT (generally to within a factor of 2 and always within a factor of 4). By contrast, isoproturon was detected in water leaving the site during periods when rapid throughflow was not predicted to be the domi-

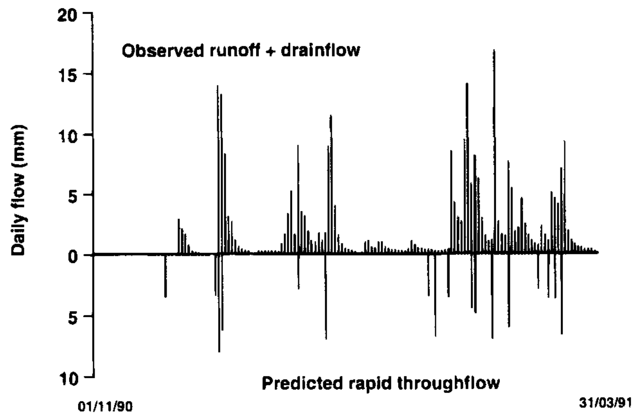

Fig. 3. Comparison between combined daily losses of surface-layer flow and mole drainflow at Cockle Park for the period 01/11/90 to 21/03/91 and losses of rapid throughflow predicted by SWAT.

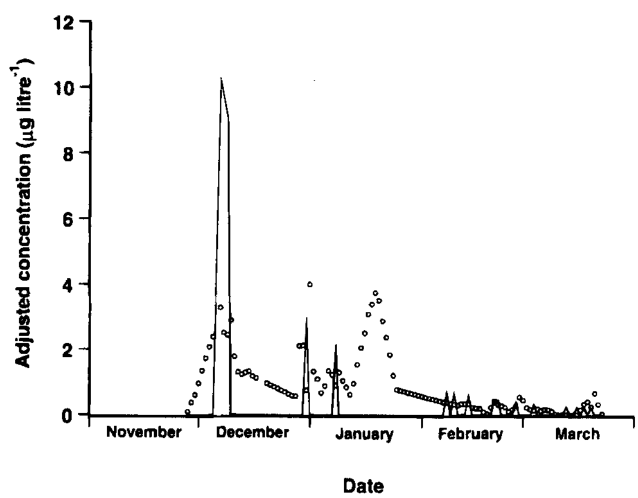

Fig. 4. Comparison between (○) observed concentrations of isoproturon adjusted to reflect total impact on surface waters from the mole-drained plot at Cockle Park during winter 1990/91 and (——) those predicted by SWAT.

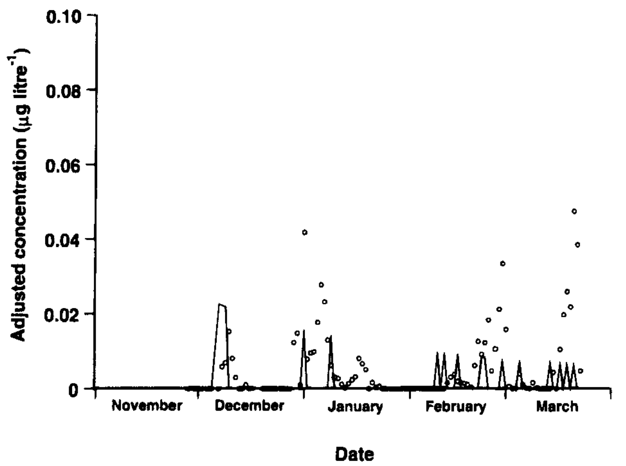

Fig. 5. Comparison between (○) observed concentrations of trifluralin adjusted to reflect total impact on surface waters from a mole-drained plot at Cockle Park during winter 1990/91 and (——) those predicted by SWAT.

nant flow pathway, reflecting the possibility that this more mobile pesticide can be transported by water moving more slowly through soil. The event which was not predicted by the model in mid-January was again important for losses of pesticide from the site. Otherwise, peaks in isoproturon concentrations did coincide with the events predicted by SWAT and their magnitude was again well predicted. Concentrations of isoproturon in the first event after application were over-predicted by a factor of 3, but the decrease in observed concentrations at Cockle Park over the course of the winter was very well described by the model.

5 CONCLUSIONS

In developing and using mathematical models, it is important to consider the purpose of the modelling exercise and any limitations which availability of data and time may impose upon model complexity. SWAT has been specifically developed to be applicable to a wide range of situations and to facilitate prediction at relatively broad scales, an approach which necessitates the adoption of a number of simplifying assumptions. The comparisons presented between field data and model predictions indicate that SWAT can be used to predict maximum concentrations of pesticide moving from a given soil to surface waters at a given point in time to within an order of magnitude. At the larger scale, there are considerable uncertainties associated with input data and these, together with the simplifying assumptions within the model, mean that SWAT should not be used to predict absolute concentrations of pesticides in surface water sources. However, the model does offer the potential to assess the likelihood of contamination of surface waters by a given compound in a given situation and as such could provide a useful tool for planning, management and regulatory purposes which complements the range of established models available to predict pesticide movement to water bodies.

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REFERENCES

1. Mullins, J. A., Carsel, R. F., Scarborough, J. E. & Ivery, A. M., PRZM-2, a model for predicting pesticide fate in the crop root and unsaturated soil zones: users manual for Release 2.0. *United States Environmental Protection Agency, Document EPA/600/R-93/046*, Athens, GA 30605-2720, 1993.
2. Leonard, R. A., Knisel, W. G. & Still, D. A., GLEAMS: Groundwater Loading Effects of Agricultural Management Systems. *Trans. ASAE*, **30** (1987) 1403–18.
3. Kladivko, E. J., Van Scouoc, G. E., Monke, E. J., Oates, K. M. & Pask, W., Pesticide and nutrient movement into subsurface tile drains on a silt loam soil in Indiana. *J. Environ. Qual.*, **20** (1991) 264–70.
4. Harris, G. L., Bailey, S. W. & Mason, D. J., The determination of pesticide losses to water courses in an agricultural clay catchment with variable drainage and land management. In *Proc. Brighton Crop Prot. Conf.—Weeds, 1991*, **3**, British Crop Protection Council, Farnham, Surrey, 1991, pp. 1271–8.
5. Brown, C. D., Carter, A. D. & Hollis, J. M., Soils and pesticide mobility. In *Environmental Behaviour of Agrochemicals*, ed. T. R. Roberts & P. Kearney. John Wiley & Sons, Chichester, 1995, pp. 131–84.
6. Hollis, J. M., Mapping the vulnerability of aquifers and surface waters to pesticide contamination at the national/regional scale. In *Pesticides in soil and water: current perspective*, ed. A. Walker. BCPC Monograph No. 47, The Lavenham Press Limited, Lavenham, Surrey, 1992, pp. 165–74.
7. Boorman, D. B., Hollis, J. M. & Lilly, A., The production of the Hydrology of Soil Types (HOST) data set. In *Proc. Brit. Hydrological Soc. Third Nat. Hydrology Symp.* Southampton University, 16–18 September 1991.
8. Boorman, D. B., Hollis, J. M. & Lilly, A., Hydrology of Soil Types: a hydrologically-based classification of the soils of the UK. *Institute of Hydrology Report No. 126*, Wallingford, UK, 1995.
9. Hall, D. G. M., Reeve, M. J., Thomasson, A. J. & Wright, V. F., Water retention, porosity and density of field soils. *Soil Survey Technical Monograph No. 9*, Harpenden, 1977.
10. Addiscott, T. M., A simple computer model for leaching in structured soils. *J. Soil Sci.*, **2** (1977) 554–63.
11. Walker, A., Evaluation of a simulation model for prediction of herbicide movement and persistence in soil. *Weed Res.*, **27** (1987) 143–52.
12. Worthing, C. R. & Hance, R. J., *The Pesticide Manual. A World Compendium. Ninth Edition.* The British Crop Protection Council, Farnham, Surrey, 1991.

13. Wauchope, R. D., Buttler, T. M., Hornsby, A. G., Augustijn-Beckers, P. W. M. & Burt, J. P., *Rev. Environ. Contam. Toxicol.*, **123**, Springer-Verlag, New York, 1992.
14. Brooke, D. & Matthiessen, P., Development and validation of a modified fugacity model of pesticide leaching from farmland. *Pestic. Sci.*, **31** (1991) 349–61.
15. Williams, R. J., Brooke, D. N., Matthiessen, P., Mills, M., Turnbull, A. & Harrison, R. M., Pesticide transport to surface waters within an agricultural catchment. *J. IWEM*, **9** (1995) 72–81.
16. Williamson, A. R. & Carter, A. D., Field studies to determine the potential risk of contamination of ground and surface waters by an autumn and spring applied herbicide in oilseed rape and fodder maize. In *Proc. Brighton Crop Prot. Conf.—Weeds, 1991*, **2**, British Crop Protection Council, Farnham, Surrey, 1991, pp. 477–84.
17. Williamson, A. R. & Carter, A. D., Determination of the potential for pollution of ground and surface waters by alachlor in oilseed rape and fodder maize: summary and regulatory interpretation. In *Proc. Brighton Crop Prot. Conf.—Weeds, 1993*, **2**, British Crop Protection Council, Farnham, Surrey, 1993, pp. 893–8.
18. Brown, C. D., Hodgkinson, R. A., Rose, D. A., Syers, J. K. & Wilcockson, S. J., Movement of pesticides to surface waters from a heavy clay soil. *Pestic. Sci.*, **43** (1995) 131–40.
19. Brown, C. D., Rose, D. A., Syers, J. K. & Hodgkinson, R. A., Effects of preferential flow upon the movement of pesticides and a conservative tracer from a heavy clay soil. In *Pesticide Movement to Water*, ed. A. Walker *et al.* BCPC Technical Monograph No. 62, The British Crop Protection Council, Farnham, Surrey, 1995, pp. 93–8.
20. Hollis, J. M. & Woods, S. M., The measurement and estimation of saturated soil hydraulic conductivity. *SSLRC Research Report*, Silsoe, UK, 1989.
21. Van Genuchten, M. Th., A closed form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.*, **44** (1980) 892–8.
22. Hollis, J. M., Hallett, S. H. & Keay, C. A., The development and application of an integrated database for modelling the environmental fate of herbicides. In *Proc. Brighton Crop Prot. Conf.—Weeds, 1993*, **3**, British Crop Protection Council, Farnham, Surrey, 1993, pp. 1355–64.
23. Carter, A. D., Vulnerability assessments and their relevance in determining the risk of herbicide contamination of water sources. *Asp. Appl. Biol.*, **29** (1992) 17–24.
24. Brown, C. D. & Hollis, J. M., Assessing the environmental impact of pesticides—a sequential modelling technique to interpret and extrapolate laboratory and field data. In *Proc. Brighton Crop Prot. Conf.—Pests and Diseases, 1994*, **2**, British Crop Protection Council, Farnham, Surrey, 1994, pp. 645–52.